

ABSTRACT

Computer-implemented methods and apparatus implementing a hierarchical protocol using multiscale molecular dynamics and molecular modeling methods to predict the structure of transmembrane proteins such as G-Protein Coupled Receptors, and protein structural models generated according to the protocol. The protocol features a combination of coarse grain sampling methods, such as hydrophobicity analysis, followed by coarse grain molecular dynamics and atomic level molecular dynamics, including accurate continuum solvation, to provide a fast and accurate procedure for predicting GPCR tertiary structure.

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